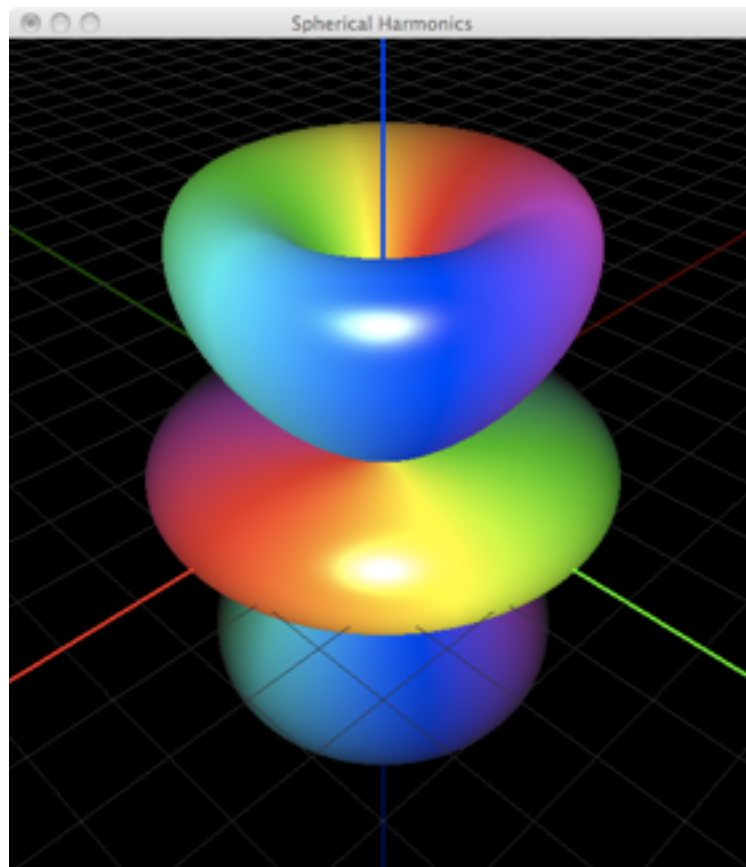


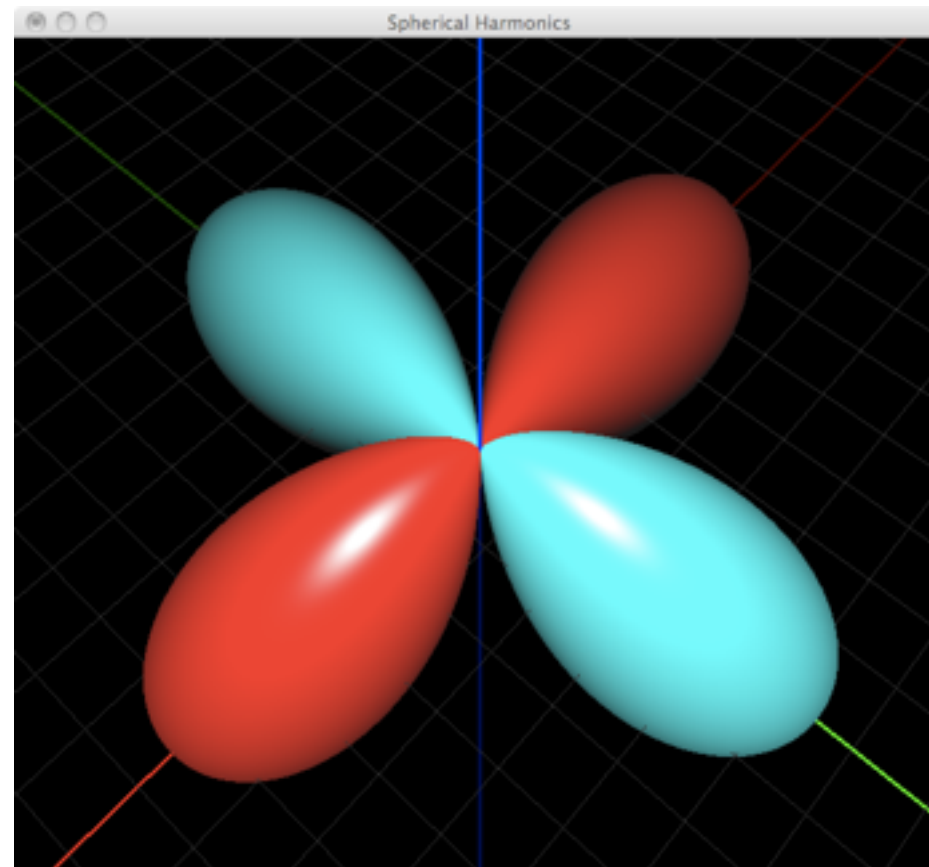
Visualizing Complex Functions using GPUs

Jülich Supercomputing Centre Guest Student Programme 2012

www.cond-mat.de/teaching/JSC/GSP12/



$Y_{3,1}$

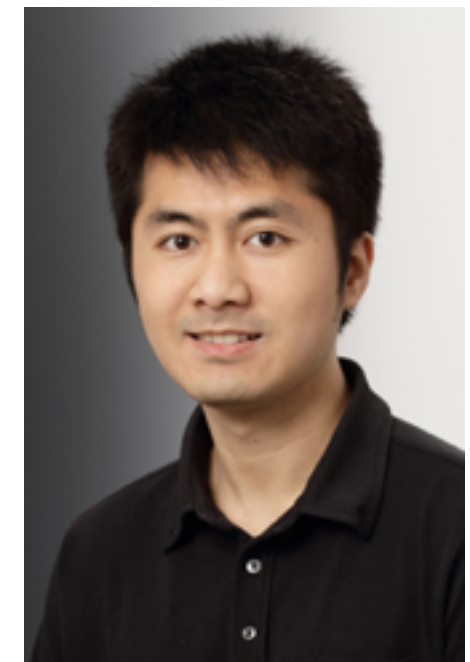
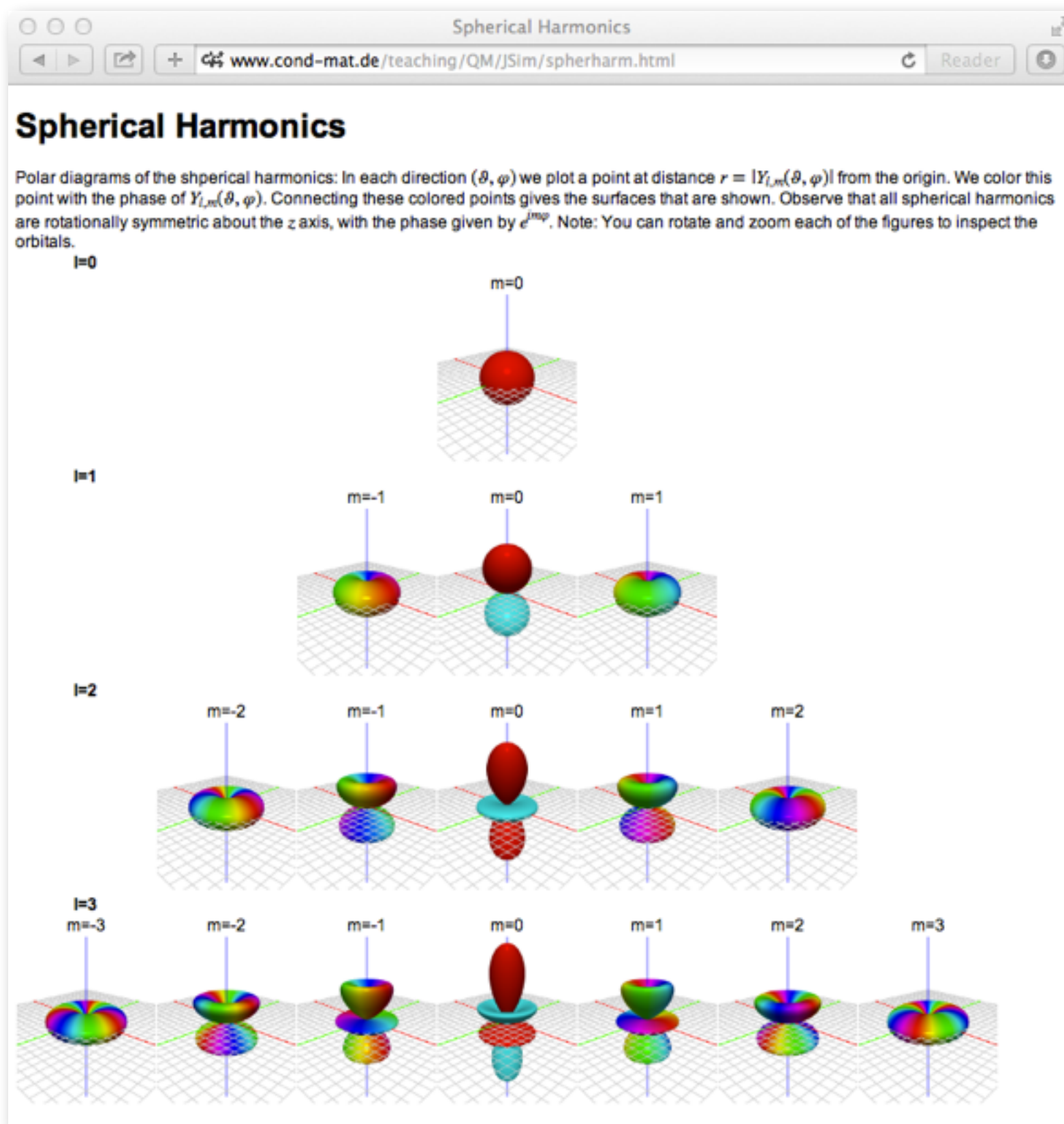


$d_{x^2-y^2}$



Khaldoon
Ghanem

interactive web page



Qian Zhang

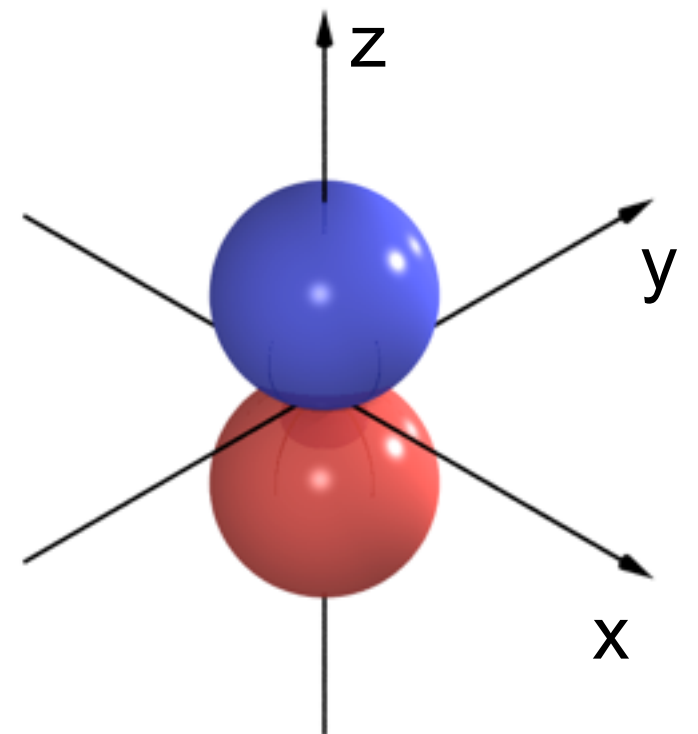
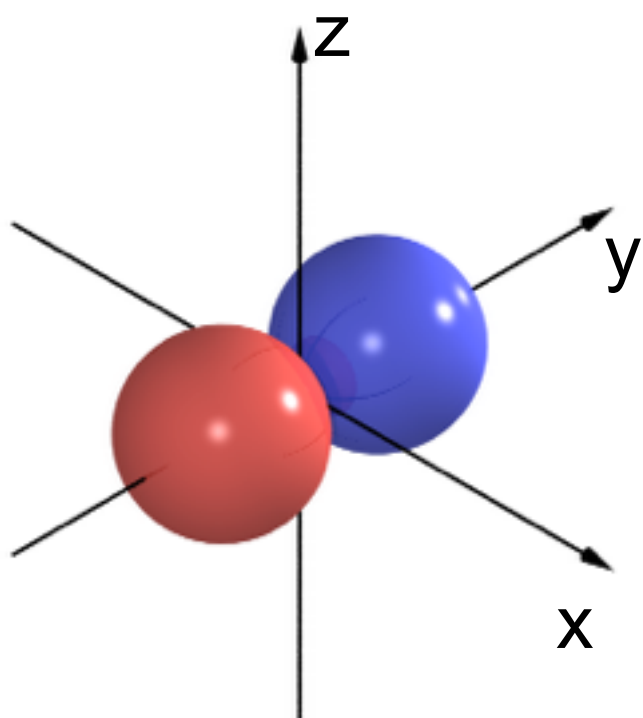
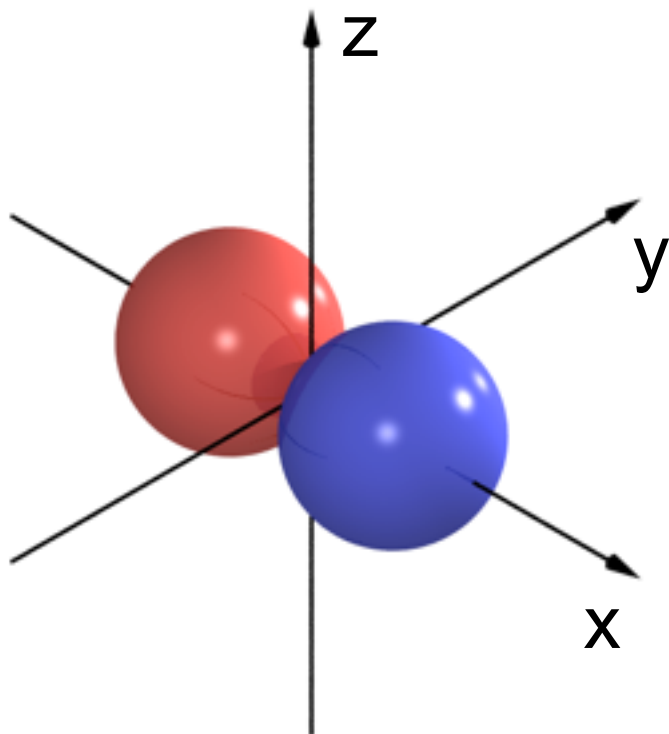
p-orbitals ($l=1$)

real orbitals

$$p_z = Y_{1,0}$$

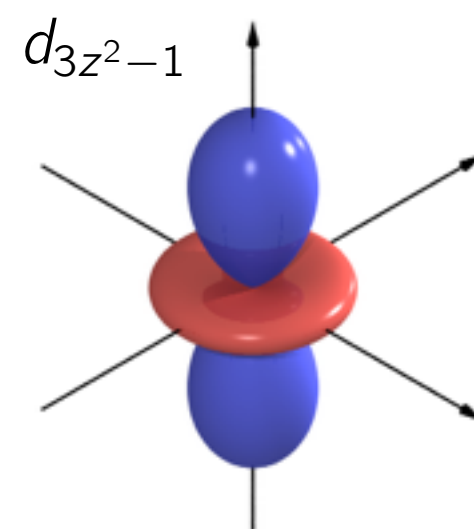
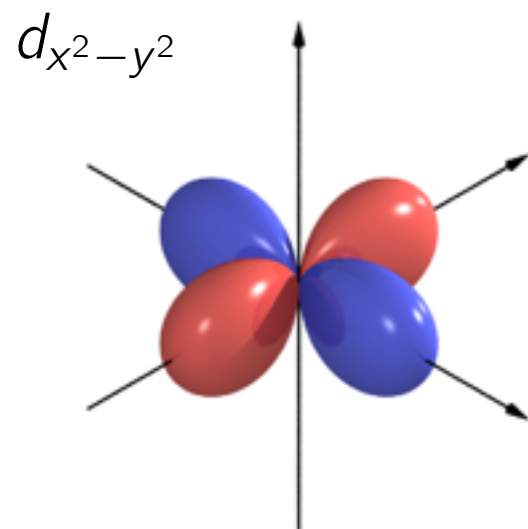
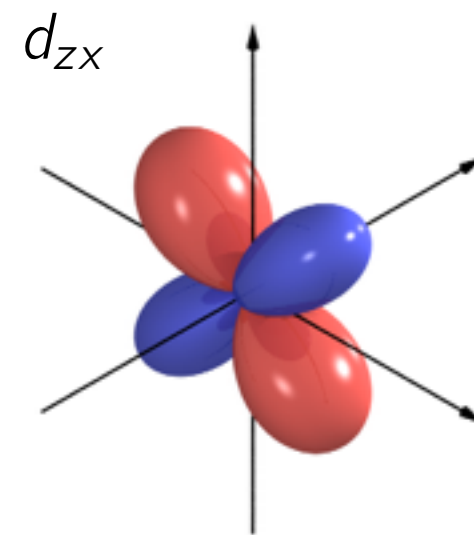
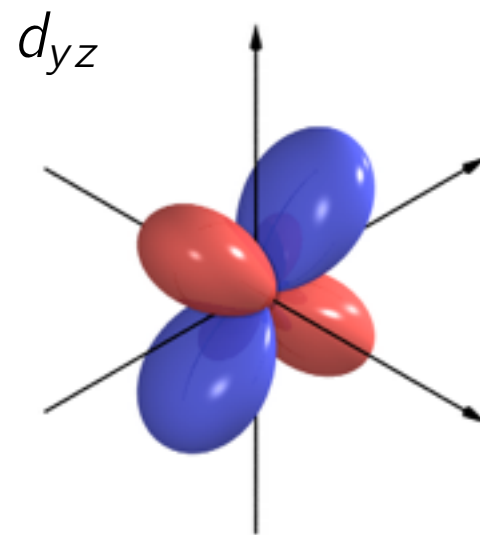
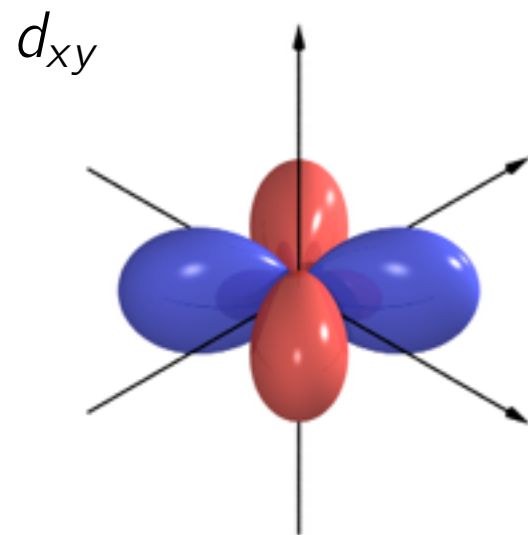
$$p_x = \sqrt{\frac{1}{2}}(Y_{1,-1} - Y_{1,1})$$

$$p_y = \sqrt{\frac{1}{2}}i(Y_{1,-1} + Y_{1,1})$$



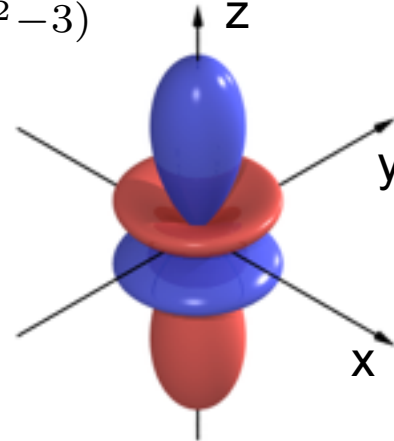
d-orbitals (*l*=2)

d_{3z^2-1}	$Y_{2,0}$	$\sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1)$
d_{zx}	$\sqrt{\frac{1}{2}} (Y_{2,-1} - Y_{2,1})$	$\sqrt{\frac{15}{16\pi}} \sin 2\theta \cos \phi$
d_{yz}	$\sqrt{\frac{1}{2}} i (Y_{2,-1} + Y_{2,1})$	$\sqrt{\frac{15}{16\pi}} \sin 2\theta \sin \phi$
d_{xy}	$\sqrt{\frac{1}{2}} i (Y_{2,-2} - Y_{2,2})$	$\sqrt{\frac{15}{16\pi}} \sin^2 \theta \cos \phi$
$d_{x^2-y^2}$	$\sqrt{\frac{1}{2}} (Y_{2,-2} + Y_{2,2})$	$\sqrt{\frac{15}{16\pi}} \sin^2 \theta \sin \phi$

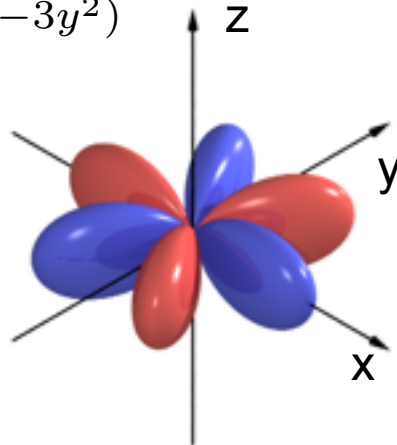


f-orbitals

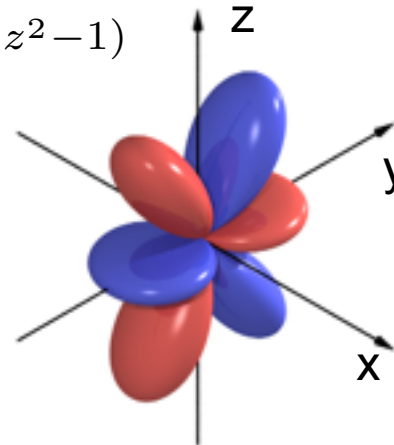
$$f_z(5z^2 - 3)$$



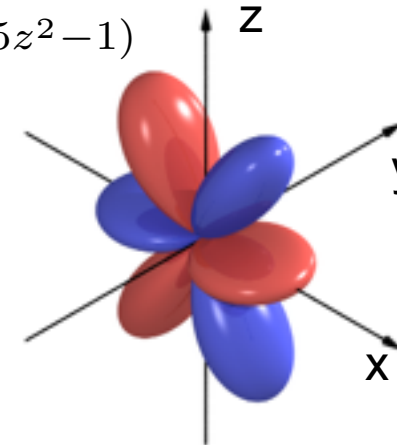
$$f_x(x^2 - 3y^2)$$



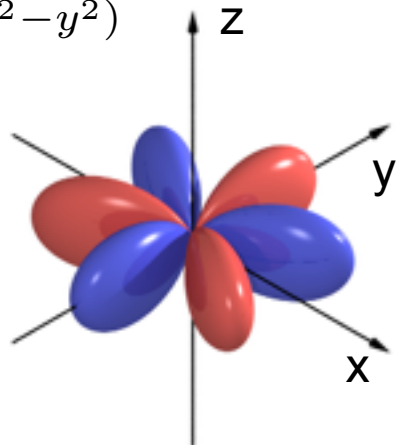
$$f_y(5z^2 - 1)$$



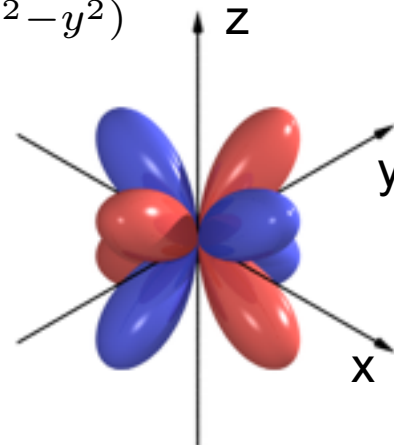
$$f_x(5z^2 - 1)$$



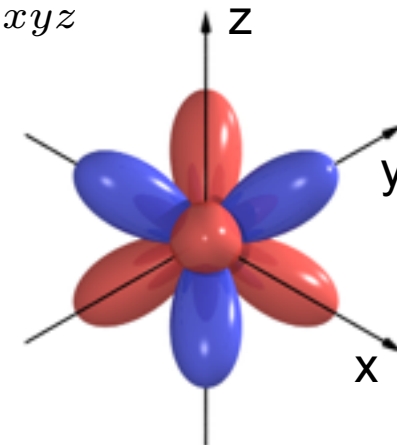
$$f_y(3x^2 - y^2)$$



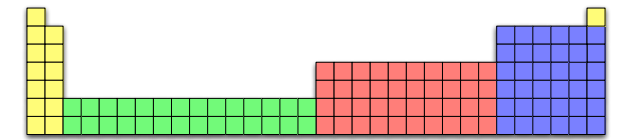
$$f_z(x^2 - y^2)$$



$$f_{xyz}$$



Periodic Table



H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	● Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	●● Lr	Rf	Db	Sg	Bh	Hs	Mt									

● La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
●● Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No

A simplified periodic table diagram. The elements are represented by colored squares. The first two columns (alkali and alkaline earth metals) are yellow. The next ten columns (transition metals) are green. The next six columns (main group elements) are red. The last column (noble gases) is blue. The noble gas column is only one square high, while the others are two squares high.

The diagram illustrates the filling order of atomic orbitals, categorized by color and labeled with their principal quantum number and subshell type. The orbitals are arranged in a grid-like structure, with the number of orbitals in each subshell indicated by the number of vertical lines within the colored area.

- Yellow (s orbitals):** 1s, 2s, 3s, 4s, 5s, 6s, 7s. Each s subshell contains 1 orbital.
- Red (d orbitals):** 3d, 4d, 5d, 6d. Each d subshell contains 5 orbitals.
- Blue (p orbitals):** 2p, 3p, 4p, 5p, 6p. Each p subshell contains 3 orbitals.
- Green (f orbitals):** 4f, 5f. Each f subshell contains 7 orbitals.

The filling order is indicated by black dots placed in the orbitals, following the Aufbau principle: 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p.